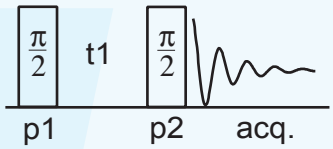
1. Introduction

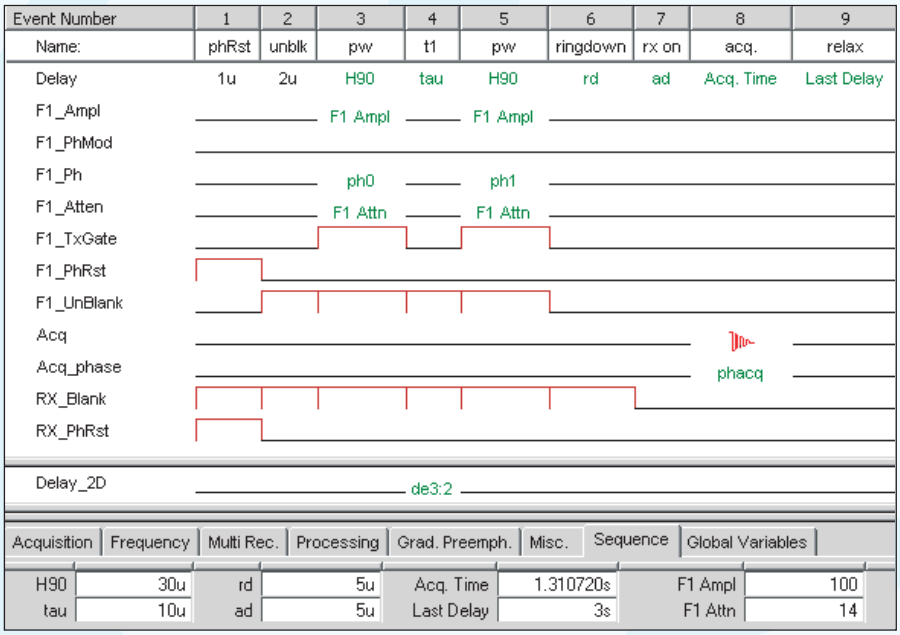
The COSY (COrrelation SpectroscopY) experiment generates 2D NMR correlation spectra. In the COSY sequence (Fig.1a), the first 90° pulse generates transverse magnetization. The second 90° pulse causes polarization transfer between J-coupled nuclei. For a two spin system with nuclei A and K, two peaks along the diagonal, (ω_A, ω_A) and (ω_K, ω_K), are observed if they are not J-coupled. If they are J-coupled, two additional cross-peaks appear at (ω_A, ω_K) and (ω_K, ω_A). Since coupled protons are typically separated by two or three covalent bonds the chemical structure can be derived from COSY spectra. Described here is the basic COSY technique and phase cycling for magnitude processing. This example demonstrates the basic principle of 2D NMR data acquisition and processing on Tecmag spectrometers.

2. Pulse sequence

(a)



(b)



1D phase tables:

ph0(P1): 0, 0, 0, 0,
1, 1, 1, 1,
2, 2, 2, 2,
3, 3, 3, 3.

ph1(P2): 0, 1, 2, 3.

phacq: 0, 2, 0, 2,
(Receiver) 3, 1, 3, 1,
2, 0, 2, 0,
1, 3, 1, 3.

(All entries are in 4 step mode.)

2D delay table:

de3:2 (t1): Auto,
Use Dwell Time,
Every Pass.

Fig. 1. (a) The pulse sequence for the COSY experiment. (b) The sequence in the NTNMR sequence editor with phase tables set for magnitude processing. The 2D delay table, "de3:2", is used for t1 increments. The t1 values are 1dw, 2dw, ..., ndw, where dw is the dwell time and n is the number in Points 2D.

3. Experiment

Sample:	2,3-dibromopropionic acid in benzene-D_6
Spectrometer:	7 Tesla magnet with Tecmag HF3 Discovery
Probe:	Nalorac D300-5 OWB 5mm $_1$H/$_{13}$C Switchable probe
90° pulse:	30 µs
SW +/- (1D) :	390.6 Hz
SW 2D:	390.6 Hz

3. Experiment (continued)

Dwell time (1D):	1.28 ms
Dwell_2D:	1.28 ms
Acq. points (and Points 1D):	1024
Points 2D:	512
Scans 1D:	4

Notes:
The sample is not spun. The magnet is shimmed to ~0.5 Hz line width. If the magnet drift is greater than 0.5 Hz during the experiment, the sample should be locked. For best results, use at least 4 scans to incorporate phase cycle on the second pulse (P2).

4. Results

Data processing:
In the NDFT window,
click the "1D" tab and select:
"Use 1D settings",
"Fourier Transform",
"Sine Bell, SB Shift: 90,
SB Skew: 5, SB width: 1024";
click the "2D" tab and select:
"Use 2D settings",
"Zero fill, 1",
"Sine Bell, SB Shift: 90,
SB Skew: 5, SB width: 1024";
"Fourier Transform",
"Transpose: complex",
click "Do it".

Display:
Click the 2D Display button,choose magnitude data and contour plot. Set the central peak to 3.4 ppm on both axes. Ramped color. Adjust zoom, axis ticks, etc.

The data processing procedure is automated in an NMRScript. To use the script, click "Scripts|Processing scripts| Process 2D (Magnitude)".

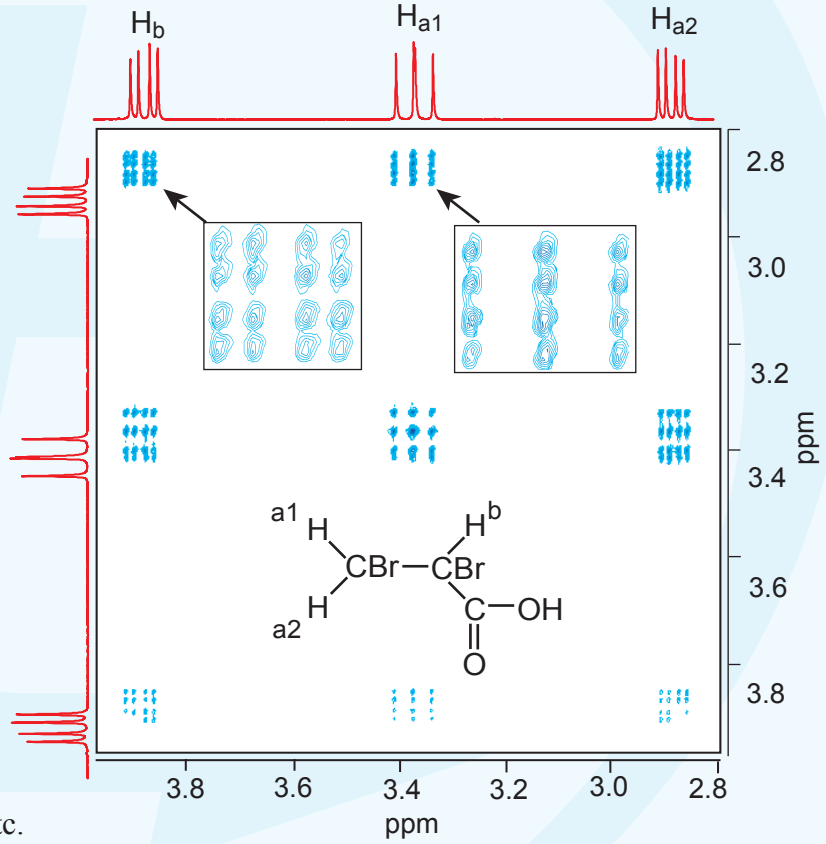


Fig. 2. Magnitude plot of the COSY spectrum of 2,3-dibromopropionic acid (only H_a and H_b are shown.). A 1D spectrum acquired with a single 90° pulse is shown on top and left sides.

5. References

1. W.P. Aue, E. Bartholdi, R.R. Ernst, *J. Chem. Phys.*, **1975**, *64*, 2229-2246.
2. Derome, A. E, "Modern NMR Techniques for Chemistry Research", Pergamon Press, New York, 1987, p. 203 - 208.
3. S. Braun, H.-O. Kalinowski, S. Berger, "150 and More Basic NMR Experiments" Wiley-VCH, Weinheim 1998, p. 353 - 355.